



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:00 PM GMT

PDB ID : 4NEH
Title : An internal ligand-bound, metastable state of a leukocyte integrin, α Xb2
Authors : Sen, M.; Yuki, K.; Springer, T.A.
Deposited on : 2013-10-29
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

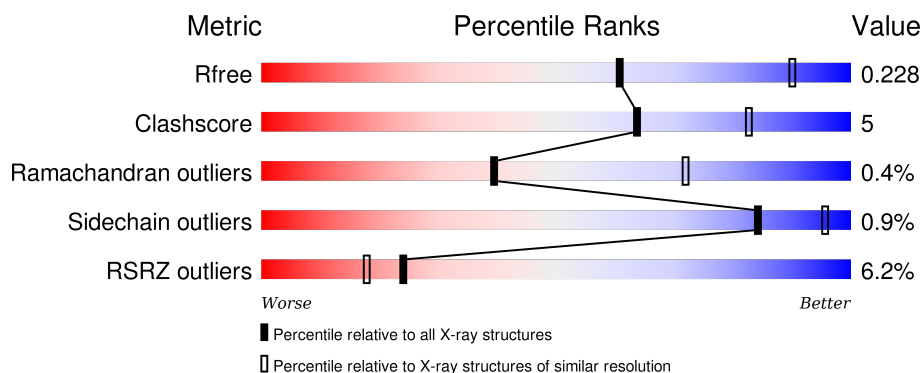
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1094	 3% 84% 14% ..
2	B	686	 10% 82% 15% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NA	A	1121	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14175 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Integrin alpha-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1084	8457	5355	1461	1602	39	0	11	1

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ASP	ASN	CONFLICT	UNP P20702
A	368	ASP	SER	CONFLICT	UNP P20702
A	678	THR	ASN	CONFLICT	UNP P20702
A	885	SER	ASN	CONFLICT	UNP P20702
A	920	CYS	ASN	CONFLICT	UNP P20702
A	1083	PRO	-	EXPRESSION TAG	UNP P20702
A	1084	GLY	-	EXPRESSION TAG	UNP P20702
A	1085	PRO	-	EXPRESSION TAG	UNP P20702
A	1086	ALA	-	EXPRESSION TAG	UNP P20702
A	1087	ALA	-	EXPRESSION TAG	UNP P20702
A	1088	LEU	-	EXPRESSION TAG	UNP P20702
A	1089	GLN	-	EXPRESSION TAG	UNP P20702
A	1090	THR	-	EXPRESSION TAG	UNP P20702
A	1091	LEU	-	EXPRESSION TAG	UNP P20702
A	1092	PHE	-	EXPRESSION TAG	UNP P20702
A	1093	GLN	-	EXPRESSION TAG	UNP P20702
A	1094	GLY	-	EXPRESSION TAG	UNP P20702

- Molecule 2 is a protein called Integrin beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	668	5153	3173	919	995	66	0	6	2

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	190	ASP	ASN	CONFLICT	UNP P05107
B	232	LYS	ASN	CONFLICT	UNP P05107
B	674	CYS	VAL	CONFLICT	UNP P05107
B	675	GLY	-	EXPRESSION TAG	UNP P05107
B	676	GLY	-	EXPRESSION TAG	UNP P05107
B	677	PRO	-	EXPRESSION TAG	UNP P05107
B	678	ALA	-	EXPRESSION TAG	UNP P05107
B	679	ALA	-	EXPRESSION TAG	UNP P05107
B	680	LEU	-	EXPRESSION TAG	UNP P05107
B	681	GLN	-	EXPRESSION TAG	UNP P05107
B	682	THR	-	EXPRESSION TAG	UNP P05107
B	683	LEU	-	EXPRESSION TAG	UNP P05107
B	684	PHE	-	EXPRESSION TAG	UNP P05107
B	685	GLN	-	EXPRESSION TAG	UNP P05107
B	686	GLY	-	EXPRESSION TAG	UNP P05107

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Ca 2 2	0	0
3	A	3	Total Ca 3 3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total C N O 28 16 2 10	0	0
5	A	2	Total C N O 28 16 2 10	0	0
5	B	2	Total C N O 28 16 2 10	0	0
5	B	2	Total C N O 28 16 2 10	0	0

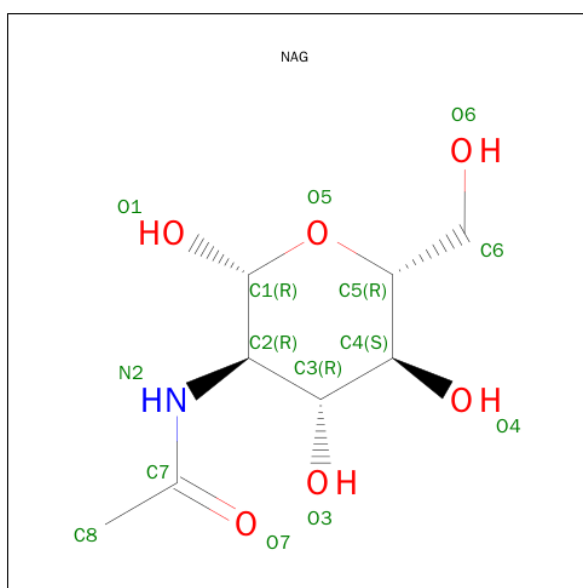
- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

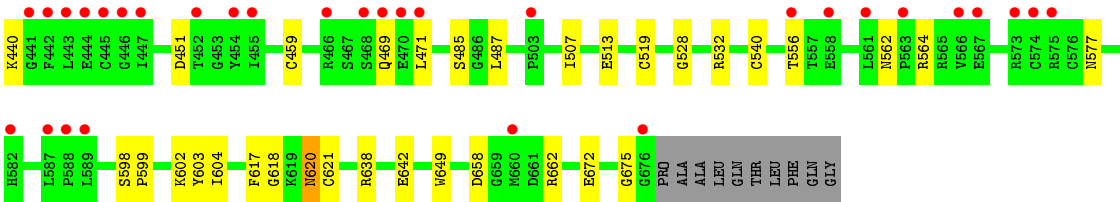
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Na 1 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	222	Total O 222 222	0	0
11	B	86	Total O 86 86	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	126.97Å 131.44Å 190.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.66 – 2.75 45.66 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.7 (45.66-2.75) 97.7 (45.66-2.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.193 , 0.225 0.196 , 0.228	Depositor DCC
R_{free} test set	4046 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.9	EDS
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 81493 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14175	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, NAG, CL, NA, CA, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/8679	0.43	3/11790 (0.0%)
2	B	0.22	0/5264	0.41	0/7103
All	All	0.22	0/13943	0.42	3/18893 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	456	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	82[A]	SER	C-N-CA	-5.11	100.53	122.00
1	A	82[B]	SER	C-N-CA	-5.11	100.53	122.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	622	GLU	Peptide
1	A	82[A]	SER	Peptide
1	A	82[B]	SER	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8457	0	8289	90	0
2	B	5153	0	4960	58	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	56	0	50	0	0
5	B	56	0	50	0	0
6	A	39	0	34	0	0
7	A	83	0	70	0	0
8	A	14	0	13	0	0
9	A	1	0	0	1	0
10	A	1	0	0	0	0
11	A	222	0	0	3	0
11	B	86	0	0	2	0
All	All	14175	0	13466	142	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (142) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:ALA:O	2:B:292:ASN:ND2	2.21	0.73
2:B:41:ASP:OD2	2:B:45:GLN:NE2	2.23	0.71
2:B:293[B]:ASN:OD1	2:B:407:ARG:NH2	2.27	0.66
1:A:723:PRO:HG3	1:A:731:ARG:HE	1.61	0.65
2:B:132:LEU:O	2:B:136:ASN:ND2	2.30	0.64
1:A:995:ILE:HG21	1:A:1040:ILE:HG23	1.81	0.62
2:B:260:ASN:O	2:B:284:GLN:NE2	2.33	0.62
1:A:12:ARG:HG2	1:A:590:GLN:HG2	1.82	0.61
1:A:318:GLU:OE1	2:B:114:SER:HB2	2.02	0.59
2:B:163:ASP:OD1	2:B:166:ARG:NH2	2.36	0.58
1:A:761:ASN:ND2	1:A:791:ASP:O	2.37	0.57
1:A:13:VAL:HG12	1:A:15:SER:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:ASP:HB2	2:B:390:GLN:HB3	1.85	0.57
2:B:658:ASP:O	2:B:662:ARG:NH1	2.38	0.57
1:A:645[B]:ASN:ND2	11:A:1366:HOH:O	2.39	0.56
1:A:669:PRO:HB3	1:A:679:ARG:HD3	1.89	0.55
2:B:618:GLY:C	2:B:620:ASN:H	2.10	0.55
1:A:307:GLN:HB2	1:A:309:GLN:HG3	1.89	0.55
1:A:159:ILE:HD12	1:A:197:LEU:HD11	1.89	0.54
1:A:342:THR:OG1	1:A:345:GLY:O	2.20	0.54
1:A:352:GLY:HA2	1:A:356:TRP:CD1	2.43	0.53
1:A:994[A]:HIS:HA	1:A:997:LYS:HE2	1.91	0.53
1:A:978:ARG:HD3	1:A:1014:ASP:HB2	1.91	0.53
1:A:469:ARG:HD3	1:A:495:GLN:HG2	1.90	0.53
2:B:231:ARG:HB2	2:B:233:VAL:HG22	1.92	0.52
2:B:82:THR:HG22	2:B:418:GLN:HB3	1.91	0.52
2:B:556:THR:HG23	2:B:577:ASN:HD21	1.75	0.52
2:B:513:GLU:N	2:B:513:GLU:OE2	2.37	0.51
1:A:479:PRO:HD3	1:A:485:TRP:CD1	2.46	0.51
1:A:71:MET:HG2	1:A:93:VAL:HG22	1.91	0.51
1:A:103:LEU:HD22	2:B:155:LEU:HB3	1.93	0.51
1:A:994[B]:HIS:HA	1:A:997:LYS:HE2	1.94	0.50
1:A:236:ILE:HG23	1:A:267:ILE:HD13	1.94	0.50
1:A:606:MET:HB2	1:A:744:ALA:HB2	1.94	0.49
2:B:434:ARG:C	2:B:436:LEU:H	2.15	0.49
1:A:134:VAL:HG22	1:A:170:SER:HB3	1.94	0.49
1:A:21:SER:OG	1:A:74:GLY:O	2.24	0.49
2:B:358:VAL:HG22	2:B:393:VAL:HG22	1.94	0.49
1:A:848:HIS:ND1	2:B:485[A]:SER:HB2	2.27	0.49
2:B:562:ASN:HD21	2:B:564:ARG:HB2	1.78	0.49
1:A:626:SER:OG	1:A:627:GLU:N	2.41	0.49
1:A:8:LEU:HD21	1:A:592:LEU:HD23	1.94	0.48
1:A:295:PHE:HZ	1:A:306:ILE:HD11	1.78	0.48
2:B:218:MET:HG2	2:B:237:LEU:HD21	1.94	0.48
1:A:602:VAL:HG22	1:A:639:ILE:HG12	1.95	0.48
1:A:372:ILE:HG12	1:A:424:TRP:CG	2.47	0.48
1:A:666:ARG:NH2	1:A:706:ASP:OD2	2.46	0.48
1:A:913:GLU:OE2	2:B:638:ARG:HB2	2.13	0.48
1:A:456:LEU:HA	1:A:477:PRO:HA	1.95	0.48
1:A:905:VAL:HG21	1:A:946:LEU:HD22	1.96	0.48
1:A:128:ARG:NH2	1:A:308:ASN:OD1	2.47	0.48
1:A:816:GLY:HA2	1:A:822:LEU:HB3	1.96	0.48
2:B:183[A]:ARG:NH2	11:B:863:HOH:O	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:MET:O	1:A:352:GLY:HA3	2.14	0.47
1:A:233:LYS:NZ	11:A:1320:HOH:O	2.31	0.47
1:A:1040:ILE:HG22	1:A:1042:GLN:H	1.79	0.47
2:B:281:SER:HB3	2:B:284:GLN:HB2	1.97	0.47
1:A:347:VAL:HG11	1:A:401:LEU:HD21	1.97	0.46
1:A:797:GLY:HA3	1:A:884:GLU:HG3	1.97	0.46
2:B:295:GLN:HG2	2:B:317:LYS:HB3	1.97	0.46
1:A:662:LEU:HD11	1:A:698:LEU:HD22	1.97	0.46
2:B:25:GLN:HG2	2:B:55:ASP:HB2	1.97	0.46
1:A:933:MET:HG2	1:A:1029:LYS:HG3	1.96	0.46
2:B:602:LYS:HE3	2:B:603:TYR:CZ	2.51	0.46
1:A:175:SER:OG	1:A:176:ASN:N	2.49	0.46
1:A:402:VAL:HG22	1:A:416:ILE:HG12	1.98	0.45
1:A:952:PHE:HB2	1:A:1011:PHE:HB2	1.97	0.45
1:A:313:LYS:NZ	1:A:331:GLU:OE2	2.35	0.45
2:B:487:LEU:HB3	2:B:507:ILE:HD13	1.96	0.45
2:B:10:SER:OG	2:B:11:CYS:N	2.49	0.45
2:B:604:ILE:HD13	2:B:642:GLU:HB2	1.97	0.45
1:A:1063:LEU:HD12	1:A:1064:PRO:HD2	1.98	0.45
1:A:629:THR:HB	1:A:700:LEU:HB2	1.99	0.45
1:A:851:PHE:HE1	1:A:857:ILE:HG12	1.82	0.45
2:B:126:LYS:NZ	2:B:130:ASP:OD2	2.41	0.45
1:A:588:ARG:NH2	11:A:1354:HOH:O	2.49	0.45
1:A:803:SER:HB3	1:A:878:THR:OG1	2.16	0.45
1:A:827:LEU:HD21	1:A:846:ILE:HG12	1.99	0.45
1:A:104:THR:OG1	1:A:105:GLY:N	2.50	0.45
2:B:433:ASP:HB3	2:B:436:LEU:HD12	2.00	0.44
1:A:513:ASN:N	1:A:513:ASN:OD1	2.51	0.44
1:A:811:ARG:HD3	1:A:864:ASP:OD2	2.17	0.44
1:A:1038:ARG:HA	1:A:1038:ARG:HD2	1.57	0.44
1:A:642:ARG:HA	1:A:642:ARG:HE	1.83	0.44
1:A:133:ILE:HG12	1:A:234:ILE:HB	2.00	0.44
1:A:812:TYR:CE2	1:A:814:ALA:HB2	2.53	0.43
2:B:178:PRO:HA	2:B:179:PRO:HD3	1.90	0.43
1:A:763:GLY:HA3	1:A:789:TRP:CE2	2.53	0.43
2:B:210:ALA:HB1	2:B:243:ASP:OD2	2.18	0.43
2:B:43:ARG:N	2:B:44:PRO:HD2	2.34	0.43
1:A:448:VAL:HA	1:A:518:THR:HB	2.01	0.43
1:A:598:PRO:HG2	1:A:732:PRO:HA	2.01	0.43
1:A:998:ASN:HA	1:A:999:PRO:HD3	1.86	0.43
2:B:110:LEU:HA	2:B:110:LEU:HD12	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:GLN:HG2	1:A:1067:GLU:HA	2.01	0.42
1:A:20:ASP:OD2	2:B:257:LEU:HD12	2.19	0.42
2:B:158:VAL:HG22	2:B:207:ASN:HB2	2.02	0.42
1:A:683:ARG:NE	1:A:694:GLU:OE2	2.29	0.42
2:B:528:GLY:HA3	2:B:532:ARG:HD2	2.01	0.42
1:A:342:THR:HA	1:A:392:LEU:HD22	2.00	0.42
2:B:42:THR:HB	2:B:44:PRO:HD2	2.01	0.42
1:A:317:ILE:HD11	2:B:170:PRO:HD3	2.00	0.42
2:B:103:TYR:O	2:B:139:THR:HG23	2.19	0.42
1:A:597:ARG:NH2	1:A:733:MET:HB3	2.33	0.42
1:A:872:GLY:H	1:A:903:TYR:HH	1.66	0.42
2:B:519:CYS:HB3	2:B:540:CYS:SG	2.60	0.42
1:A:131:GLN:HG3	1:A:167:THR:HG23	2.01	0.42
2:B:9:SER:OG	2:B:13:GLU:OE1	2.31	0.42
1:A:419:GLN:HG3	1:A:424:TRP:CE2	2.54	0.42
2:B:469:GLN:C	2:B:471:LEU:H	2.23	0.42
2:B:104:PRO:HB2	2:B:233:VAL:HG11	2.01	0.42
2:B:109:TYR:O	2:B:146:PHE:HB2	2.19	0.42
1:A:447:ASP:OD2	1:A:450:SER:HA	2.20	0.42
2:B:11:CYS:O	2:B:15:ILE:HG12	2.20	0.41
1:A:670:ARG:NH1	1:A:709:THR:O	2.41	0.41
2:B:437:CYS:O	2:B:459:CYS:HB2	2.20	0.41
1:A:295:PHE:CZ	1:A:306:ILE:HD11	2.55	0.41
1:A:132:ASP:HB3	1:A:184:PHE:CZ	2.56	0.41
2:B:225:PRO:HA	2:B:230:TRP:HD1	1.86	0.41
1:A:660:LEU:HD21	1:A:715:LEU:HD12	2.01	0.41
2:B:34:ASP:HA	2:B:35:PRO:HD3	1.82	0.41
1:A:111:GLY:HA2	1:A:112:PRO:HD3	1.92	0.41
2:B:649:TRP:HB2	2:B:672:GLU:HB2	2.02	0.41
2:B:362:SER:HB2	2:B:370:HIS:HB2	2.02	0.41
1:A:832:ALA:HA	1:A:833:PRO:HD3	1.86	0.41
2:B:617:PHE:HA	2:B:620:ASN:HB3	2.03	0.41
1:A:137:ILE:HG22	1:A:238:ILE:HD12	2.02	0.41
2:B:440:LYS:HB3	2:B:451:ASP:OD2	2.21	0.41
1:A:11:PHE:CE1	1:A:50:CYS:HB3	2.56	0.41
2:B:107:LEU:HB2	2:B:135:LEU:HD13	2.03	0.41
1:A:176:ASN:HB3	1:A:206:PHE:HB2	2.03	0.40
1:A:9:THR:HB	1:A:593:LEU:HB3	2.02	0.40
1:A:613:ILE:HG21	1:A:618[B]:PHE:CE2	2.56	0.40
1:A:364:PRO:HA	1:A:365:PRO:HD3	1.95	0.40
2:B:598:SER:HA	2:B:599:PRO:HD3	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:ARG:HA	1:A:618[A]:PHE:CE1	2.57	0.40
1:A:613:ILE:HG21	1:A:618[B]:PHE:HE2	1.87	0.40
2:B:375:ARG:HD3	11:B:848:HOH:O	2.21	0.40
1:A:140:SER:HB2	9:A:1120:CL:CL	2.59	0.40
2:B:106:ASP:OD1	2:B:143:ARG:HB2	2.21	0.40
1:A:368:ASP:HA	1:A:369:PRO:HD3	1.91	0.40
1:A:657:THR:HG23	1:A:684:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1093/1094 (100%)	1044 (96%)	44 (4%)	5 (0%)	34	67
2	B	668/686 (97%)	637 (95%)	29 (4%)	2 (0%)	46	77
All	All	1761/1780 (99%)	1681 (96%)	73 (4%)	7 (0%)	39	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	SER
1	A	543	PRO
2	B	621	CYS
1	A	175	SER
1	A	975	PRO
2	B	675	GLY
1	A	999	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	932/932 (100%)	927 (100%)	5 (0%)	92	97
2	B	582/590 (99%)	573 (98%)	9 (2%)	72	92
All	All	1514/1522 (100%)	1500 (99%)	14 (1%)	84	95

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	TRP
1	A	438	TYR
1	A	642	ARG
1	A	894	THR
1	A	1038	ARG
2	B	103	TYR
2	B	124	VAL
2	B	171	ASN
2	B	172	LYS
2	B	173	GLU
2	B	207	ASN
2	B	267	GLU
2	B	281	SER
2	B	620	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	399	GLN
1	A	912	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

18 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	NAG	A	1105	1,5	14,14,15	0.60	0	15,19,21	0.42	0
5	NAG	A	1106	5	14,14,15	0.29	0	15,19,21	0.30	0
6	NAG	A	1107	1,6	14,14,15	0.21	0	15,19,21	0.43	0
6	NAG	A	1108	6	14,14,15	0.23	0	15,19,21	0.52	0
6	BMA	A	1109	6	11,11,12	0.67	0	14,15,17	1.69	3 (21%)
7	NAG	A	1110	1,7	14,14,15	0.84	1 (7%)	15,19,21	0.38	0
7	NAG	A	1111	7	14,14,15	0.22	0	15,19,21	0.25	0
7	BMA	A	1112	7	11,11,12	0.85	1 (9%)	14,15,17	1.13	1 (7%)
7	MAN	A	1113	7	11,11,12	0.70	0	14,15,17	1.29	3 (21%)
7	MAN	A	1114	7	11,11,12	0.79	1 (9%)	14,15,17	1.20	3 (21%)
7	MAN	A	1115	7	11,11,12	0.59	0	14,15,17	1.41	3 (21%)
7	MAN	A	1116	7	11,11,12	0.69	0	14,15,17	1.10	1 (7%)
5	NAG	A	1117	1,5	14,14,15	0.44	0	15,19,21	0.61	0
5	NAG	A	1118	5	14,14,15	0.52	0	15,19,21	0.48	0
5	NAG	B	704	2,5	14,14,15	0.38	0	15,19,21	0.72	1 (6%)
5	NAG	B	705	5	14,14,15	0.40	0	15,19,21	0.45	0
5	NAG	B	706	2,5	14,14,15	0.35	0	15,19,21	0.55	0
5	NAG	B	707	5	14,14,15	0.35	0	15,19,21	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1105	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1106	5	-	0/6/23/26	0/1/1/1
6	NAG	A	1107	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1108	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1109	6	-	0/2/19/22	0/1/1/1
7	NAG	A	1110	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1111	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1112	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1113	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1114	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1115	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1116	7	-	0/2/19/22	0/1/1/1
5	NAG	A	1117	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1118	5	-	0/6/23/26	0/1/1/1
5	NAG	B	704	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	705	5	-	0/6/23/26	0/1/1/1
5	NAG	B	706	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	707	5	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1110	NAG	O5-C1	-3.06	1.38	1.43
7	A	1112	BMA	O5-C1	-2.08	1.40	1.43
7	A	1114	MAN	C1-C2	2.15	1.57	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1114	MAN	O2-C2-C3	-2.31	105.48	110.12
6	A	1109	BMA	O2-C2-C3	-2.28	105.52	110.12
7	A	1115	MAN	O2-C2-C3	-2.23	105.64	110.12
7	A	1113	MAN	O2-C2-C3	-2.13	105.84	110.12
7	A	1115	MAN	C1-C2-C3	-2.04	107.12	109.54
7	A	1114	MAN	C1-C2-C3	2.19	112.14	109.54
7	A	1114	MAN	C1-O5-C5	2.36	115.24	112.25
7	A	1113	MAN	O3-C3-C2	2.39	114.32	110.00
5	B	704	NAG	C1-O5-C5	2.48	115.39	112.25
7	A	1116	MAN	C1-O5-C5	2.60	115.54	112.25
7	A	1112	BMA	C1-O5-C5	2.81	115.81	112.25
7	A	1113	MAN	C1-O5-C5	2.84	115.86	112.25
6	A	1109	BMA	O5-C1-C2	2.84	115.47	110.86
7	A	1115	MAN	C1-O5-C5	3.54	116.75	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1109	BMA	C1-O5-C5	4.06	117.40	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	A	1119	1	14,14,15	0.56	0	15,19,21	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1119	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1084/1094 (99%)	0.23	37 (3%) 49 42	40, 70, 143, 274	0
2	B	668/686 (97%)	0.54	72 (10%) 8 5	43, 90, 168, 230	1 (0%)
All	All	1752/1780 (98%)	0.35	109 (6%) 24 18	40, 76, 159, 274	1 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	624	VAL	10.1
1	A	625	VAL	8.3
1	A	888	PRO	7.0
2	B	561	LEU	7.0
2	B	469	GLN	6.8
2	B	73	GLN	6.7
1	A	890	THR	5.8
1	A	618[A]	PHE	5.6
1	A	817	GLN	5.5
2	B	468	SER	5.5
1	A	322	THR	5.4
2	B	470	GLU	5.4
2	B	427	CYS	5.4
2	B	426	ARG	5.4
2	B	434	ARG	5.4
1	A	823	ARG	5.3
1	A	836	SER	5.3
1	A	819	GLN	5.3
2	B	32	PRO	5.2
2	B	29	PHE	5.0
2	B	558	GLU	4.8
1	A	824	SER	4.7
2	B	27	LEU	4.7
2	B	50	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	753	GLY	4.4
1	A	815	GLU	4.4
1	A	820	GLY	4.3
2	B	435	SER	4.1
2	B	428	ARG	4.1
2	B	445	CYS	4.1
2	B	26	LYS	4.0
2	B	47	LEU	3.9
2	B	443	LEU	3.9
2	B	567	GLU	3.8
2	B	38	ILE	3.7
2	B	433	ASP	3.7
1	A	623	GLN	3.6
1	A	757	ILE	3.6
1	A	838	GLY	3.5
2	B	563	PRO	3.5
1	A	621	ARG	3.4
2	B	454	TYR	3.3
2	B	442	PHE	3.3
2	B	455	ILE	3.3
1	A	719	LEU	3.2
1	A	756	HIS	3.2
2	B	438	HIS	3.2
2	B	46	LEU	3.2
2	B	28	ASN	3.2
2	B	30	THR	3.2
2	B	49	ARG	3.1
2	B	68	ASP	3.1
1	A	626	SER	3.1
1	A	720	VAL	3.1
1	A	755	ASP	3.1
2	B	587	LEU	3.0
1	A	754	ALA	3.0
2	B	423	CYS	3.0
1	A	762	LEU	2.9
1	A	740	ARG	2.9
1	A	752	CYS	2.9
2	B	437	CYS	2.9
2	B	676	GLY	2.9
2	B	446	GLY	2.9
2	B	588	PRO	2.9
2	B	92	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	51	CYS	2.8
2	B	466	ARG	2.8
2	B	471	LEU	2.8
1	A	889	ARG	2.8
2	B	1	GLN	2.7
1	A	622	GLU	2.6
1	A	821	GLN	2.6
2	B	23	TRP	2.6
2	B	503	PRO	2.6
2	B	420	LEU	2.6
2	B	660	MET	2.6
1	A	892	LYS	2.5
2	B	54	ASP	2.5
2	B	589	LEU	2.5
2	B	91	ALA	2.4
2	B	424	GLU	2.4
1	A	323	THR	2.4
2	B	53	ALA	2.4
2	B	52	ALA	2.4
2	B	573	ARG	2.3
2	B	121	LEU	2.3
2	B	363	PHE	2.3
2	B	566	VAL	2.3
2	B	347	LEU	2.3
2	B	39	ARG	2.3
1	A	282	LEU	2.3
2	B	447	ILE	2.3
2	B	444	GLU	2.3
1	A	656	VAL	2.3
2	B	441	GLY	2.3
1	A	825	LEU	2.2
2	B	574	CYS	2.2
2	B	56	ILE	2.2
2	B	575	ARG	2.2
1	A	396	LYS	2.2
2	B	425	CYS	2.2
2	B	55	ASP	2.1
2	B	33	GLY	2.1
2	B	268	ASP	2.1
2	B	556	THR	2.1
2	B	452	THR	2.1
1	A	619	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	582	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	NAG	A	1110	14/15	0.96	0.14	-0.32	37,53,61,86	0
5	NAG	B	704	14/15	0.94	0.21	-0.36	80,106,119,120	0
5	NAG	A	1117	14/15	0.95	0.16	-0.60	66,86,100,113	0
6	NAG	A	1107	14/15	0.94	0.13	-1.03	59,85,92,111	0
5	NAG	A	1106	14/15	0.89	0.17	-	85,118,155,161	0
7	BMA	A	1112	11/12	0.79	0.16	-	106,123,165,169	0
5	NAG	A	1118	14/15	0.92	0.22	-	105,127,133,139	0
7	MAN	A	1116	11/12	0.86	0.16	-	146,156,174,181	0
6	NAG	A	1108	14/15	0.88	0.19	-	90,117,135,159	0
6	BMA	A	1109	11/12	0.57	0.36	-	136,171,177,177	0
7	MAN	A	1113	11/12	0.87	0.41	-	164,171,177,183	0
5	NAG	B	706	14/15	0.94	0.20	-	100,105,121,121	0
7	MAN	A	1115	11/12	0.91	0.16	-	107,117,127,131	0
7	NAG	A	1111	14/15	0.89	0.14	-	60,85,111,121	0
5	NAG	A	1105	14/15	0.96	0.09	-	56,75,93,99	0
5	NAG	B	705	14/15	0.87	0.30	-	143,154,167,176	0
5	NAG	B	707	14/15	0.85	0.33	-	148,162,179,182	0
7	MAN	A	1114	11/12	0.72	0.42	-	158,169,191,196	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	NA	A	1121	1/1	0.90	0.40	7.61	77,77,77,77	0
3	CA	B	701	1/1	0.98	0.21	0.33	48,48,48,48	0
9	CL	A	1120	1/1	0.95	0.16	0.09	82,82,82,82	0
4	MG	B	703	1/1	0.99	0.19	-0.07	46,46,46,46	0
3	CA	A	1101	1/1	0.99	0.18	-0.24	46,46,46,46	0
3	CA	A	1103	1/1	0.99	0.12	-0.69	54,54,54,54	0
4	MG	A	1102	1/1	0.98	0.12	-0.85	69,69,69,69	0
3	CA	A	1104	1/1	0.80	0.07	-2.39	143,143,143,143	0
3	CA	B	702	1/1	0.97	0.10	-2.59	100,100,100,100	0
8	NAG	A	1119	14/15	0.74	0.45	-	152,172,178,181	0

6.5 Other polymers [i](#)

There are no such residues in this entry.